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The Spectroscopic, Molecular Structure and Electrostatic Potential, Polarizability Hyperpolarizability, and Homo–Lumo Analysis of Monomeric and Dimeric Structures of 2-Chloro-N-(2 Methylphenyl) Benzamide

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Abstract : The monomer and dimer structures of the title molecule have been obtained from density functional theory (DFT) B3LYP method with 6-31G (d,p) as basis set calculations. The optimized geometrical parameters obtained by B3LYP/6-31G (d,p) method shows good agreement with experimental X-ray data. The polarizability and first order hyperpolarizabilty of the title molecule were calculated and interpreted. The intermolecular N–H•••O hydrogen bonds are discussed in dimer structure of the molecule. The vibrational wave numbers and their assignments were examined theoretically using the Gaussian 09 set of quantum chemistry codes. The predicted frontier molecular orbital energies at B3LYP/6-31G(d,p) method set show that charge transfer occurs within the molecule. The frontier molecular orbital calculations clearly show the inverse relationship of HOMO–LUMO gap with the total static hyperpolarizability. The results also show that 2-Chloro-N-(2-methylphenyl) benzamide 2 molecule may have nonlinear optical (NLO) comportment with non-zero values.

Keywords : DFT, HOMO, LUMO, NLO
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